Using compositional geochemical ground survey data as predictors for geogenic radon potential

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Using compositional geochemical ground survey data as predictors for geogenic radon potential

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International Workshop on the European Atlas of Natural Radiation
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The International Association of Mathematical Geoscience (IAMG) and GeoMap

IAMG

This collaborative research stems from the first GeoMap Workshop (held in Olomouc, Czech Republic, 17-20 June 2014) that discussed the challenges and the usefulness of compositional data analysis (CoDA) for regional geochemistry.

The Single Component Geochemical Map: Fact or Fiction, J of Geochemical Exploration (in review)

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Premise and methods

The question:

How can ground-based geochemical data be used as predictors for geogenic radon potential?

The underlying concept:

Soil geochemical elements (e.g. K, U, Th) are related to underlying geology and natural gamma-radiation.

Geochemical data are compositional (inherently multivariate and relative in nature). They need to be analysed simultaneously.

The methodology:

Compositional geostatistical data analysis techniques and regression analysis with compositional data.

The Tellus and Tellus Border Projects

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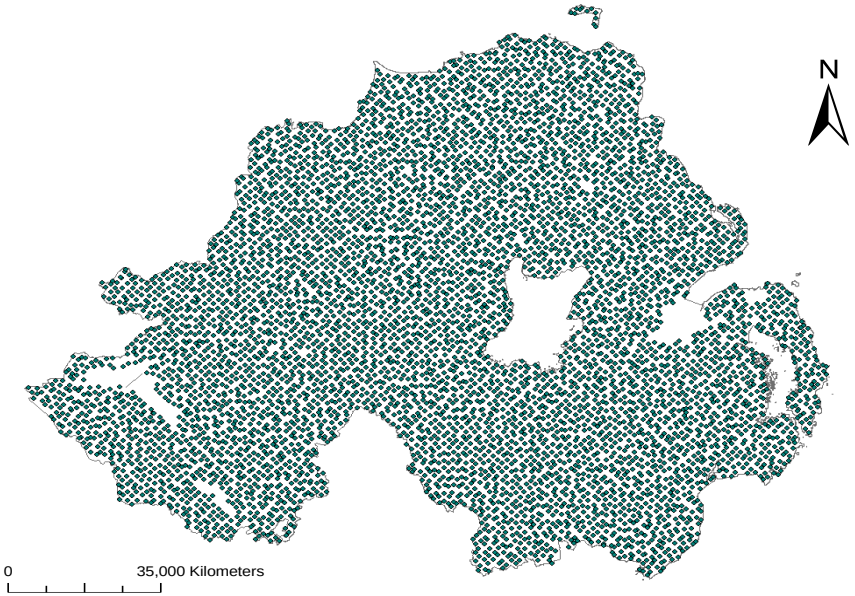
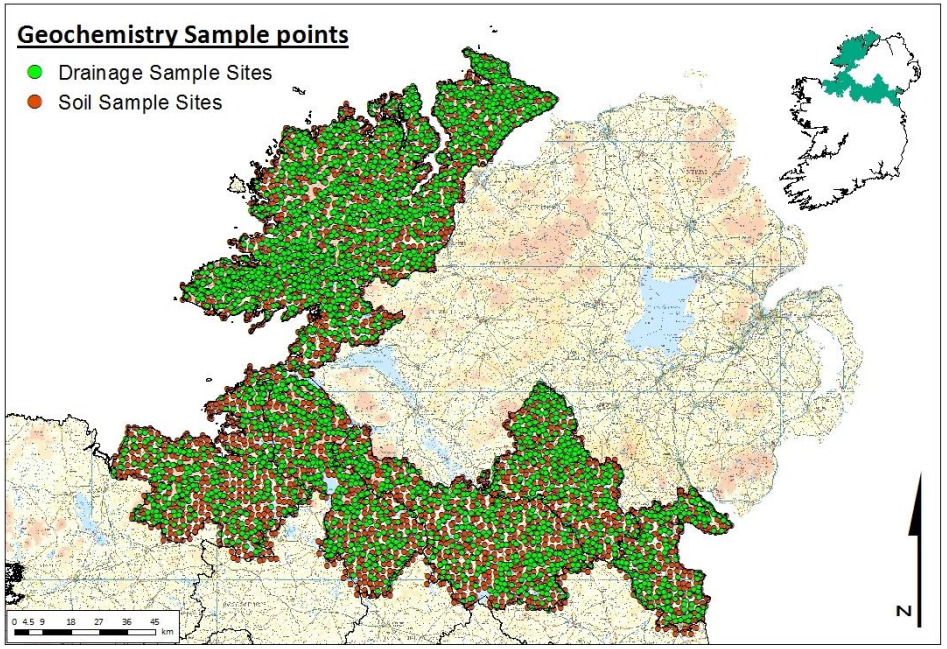
An EU INTERREG IVA-funded regional mapping project

Soil Geochemistry Sampling





www.tellusborder.eu

The Tellus Project

– Managed by the Geological Survey of Northern Ireland (GSNI) and funded by the Department of Enterprise Trade and Development

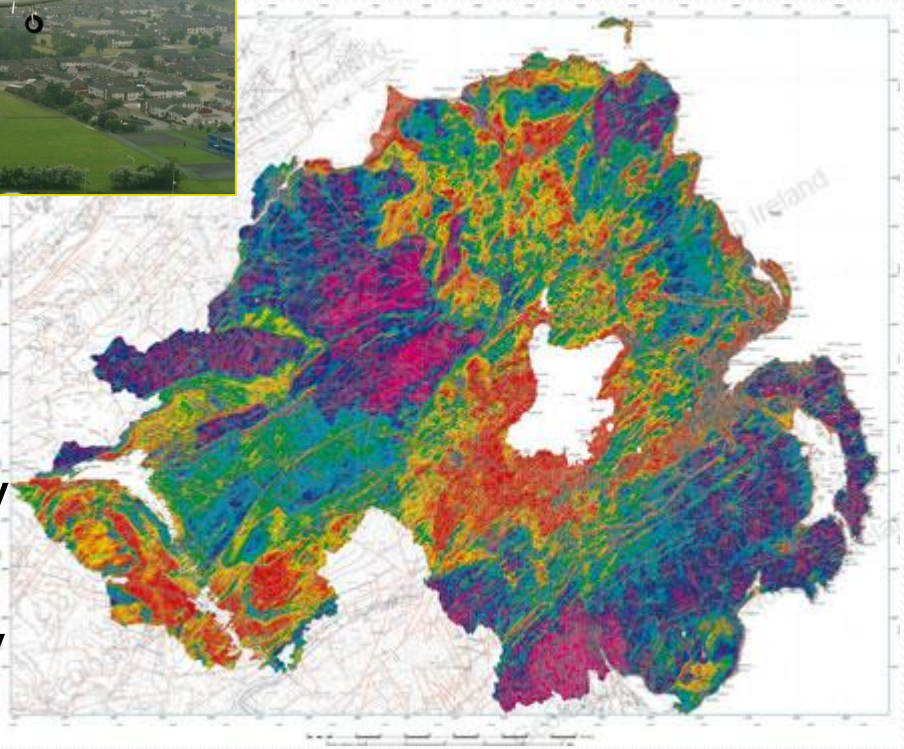
Airborne passive sensors:
using naturally available energy

- Involved the most concentrated geological mapping project ever undertaken in Northern Ireland.
- The data comprise multi-source airborne geophysics collected by a specialist survey aircraft
  - Magnetics
  - Natural radioactivity
  - Electrical Conductivity

Magnetics

Natural radioactivity

Electrical conductivity



http://www.bgs.ac.uk/gsni/tellus/map_viewer/application/magnetics_tmi.html

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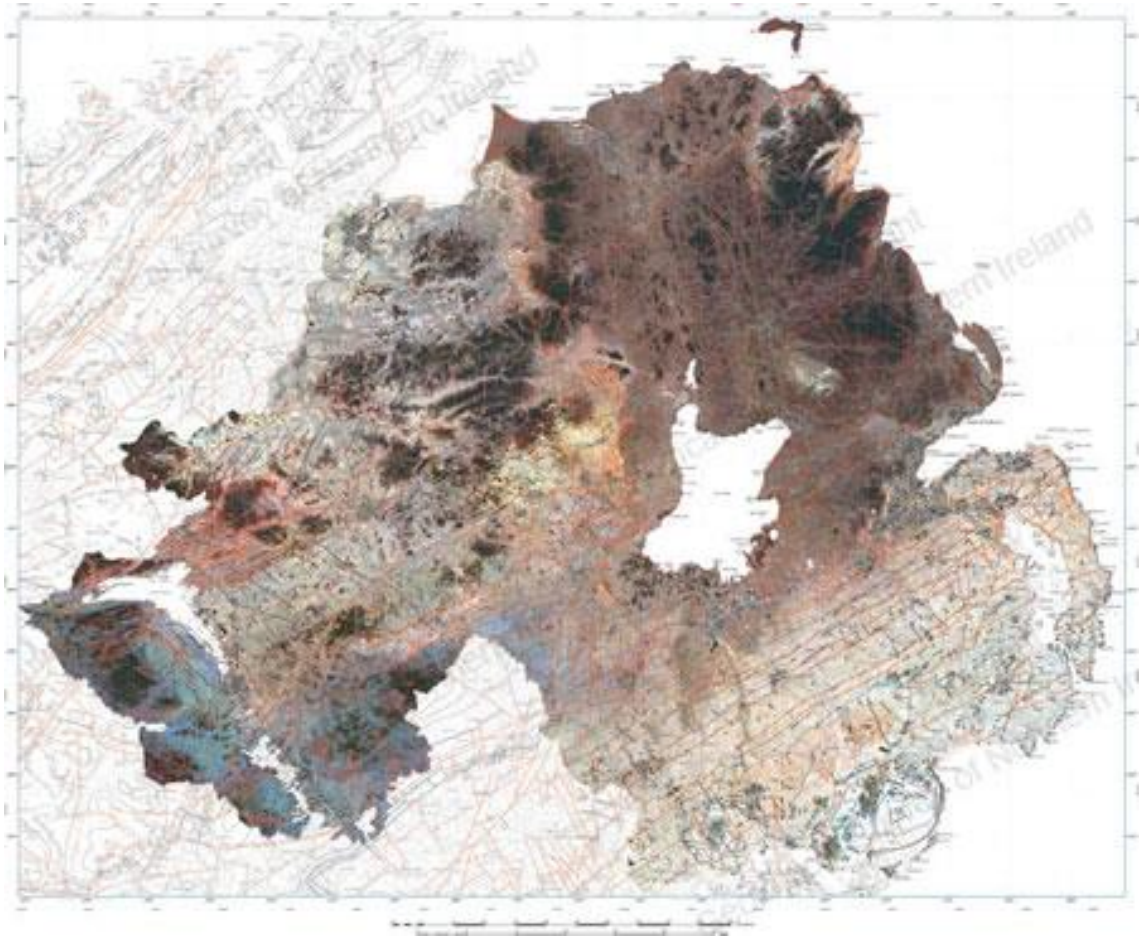
Natural radioactivity



http://www.bgs.ac.uk/gsni/tellus/map_viewer/application/magnetics_tmi.html

Single geochemical components?

- Geochemical maps are the most basic representation of spatial elemental distributions

For regional geochemistry, the key applications of the data are generally either to:

- ➢ produce and use elemental concentration maps (one-component regional distribution maps) or
- ➢ explore associations between elements affected by geological/geochemical processes.
- Used for environmental geochemistry.
- Potential for geogenic radon mapping?

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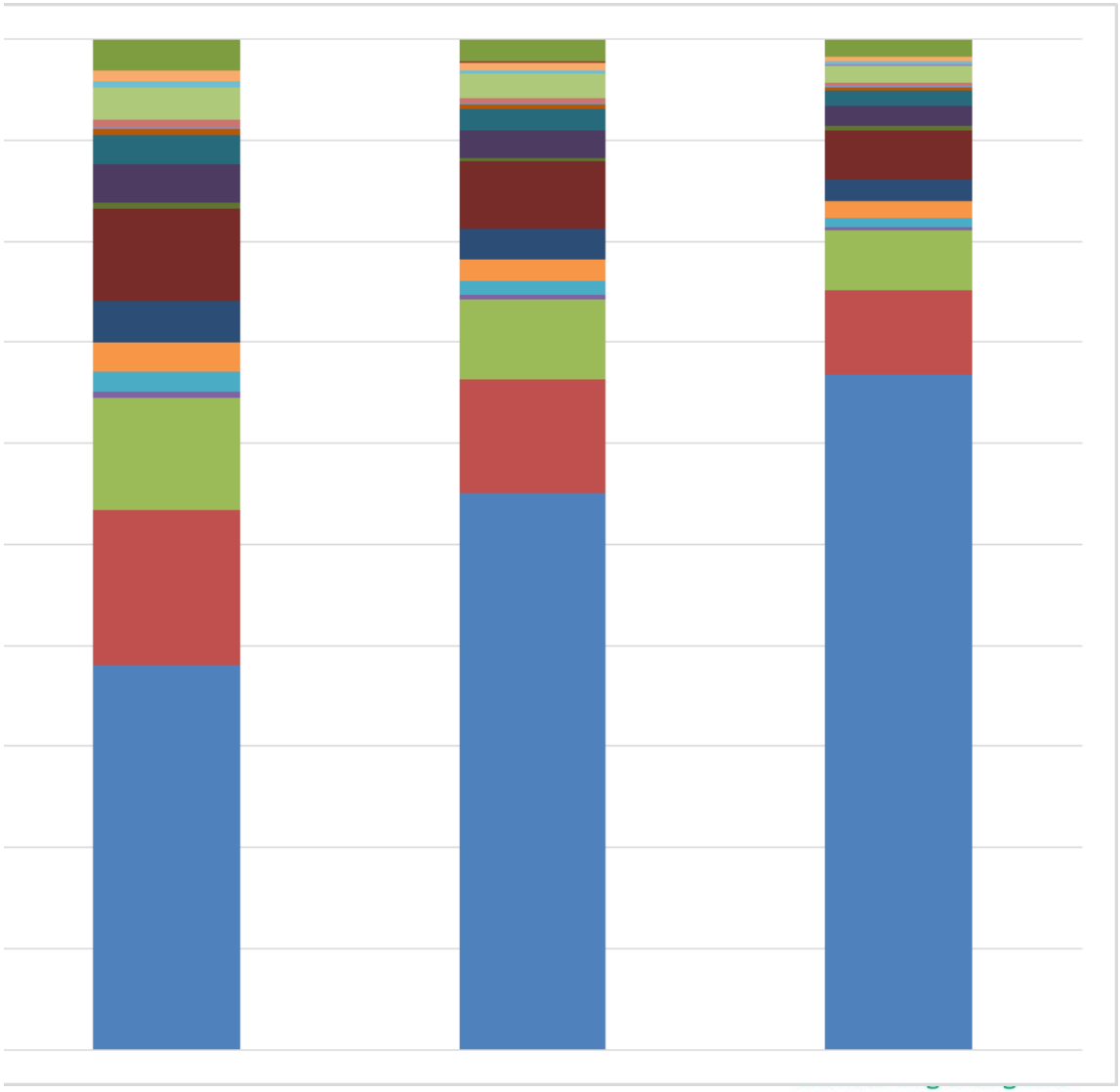
The nature of compositional data

These compositions only differ in a dilution by the blue component

The components may be reported in different physical units (ppm, mg/kg or as percentages) and all the components may not be reported or measured.

The components do not need to add up to 100%

However, each component has an amount which represents its importance as part of the whole composition.



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The nature of geochemical data

- The compositional nature imposes several limitations on how the data should be presented.
- This isn't new: Felix Chayes (1960) 'the percentage is already a complicated ratio', "closure restraint".
- Common ways used to deal with this have included the use of ternary or quaternary diagrams and to sum components to form subsets (with or without common elements).
- Unfortunately both these methods have the same effect as the initial percentages or even strengthen the closure effect (a closed ternary system).
- In general this leads to a tendency towards negative correlation between major components and may even introduce a bias towards positive correlation between minor components.

- Geochemical data constitute amounts of components with relative portions of a total even if this total is unknown.
- The constraints of constant sum or the closed nature of the relative amounts of components have implications for the analysis of geochemical data.

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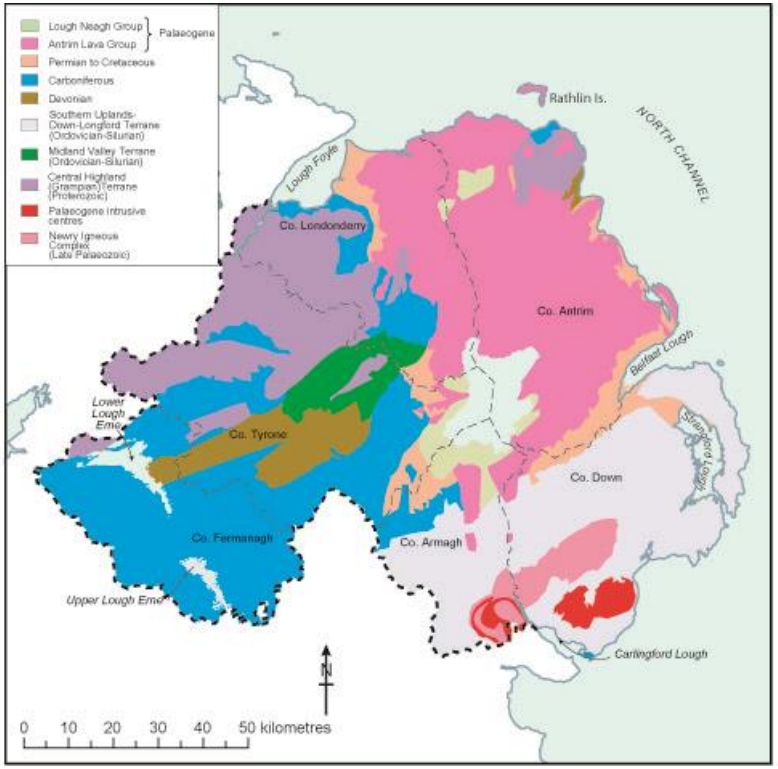
Regional scale example

A)



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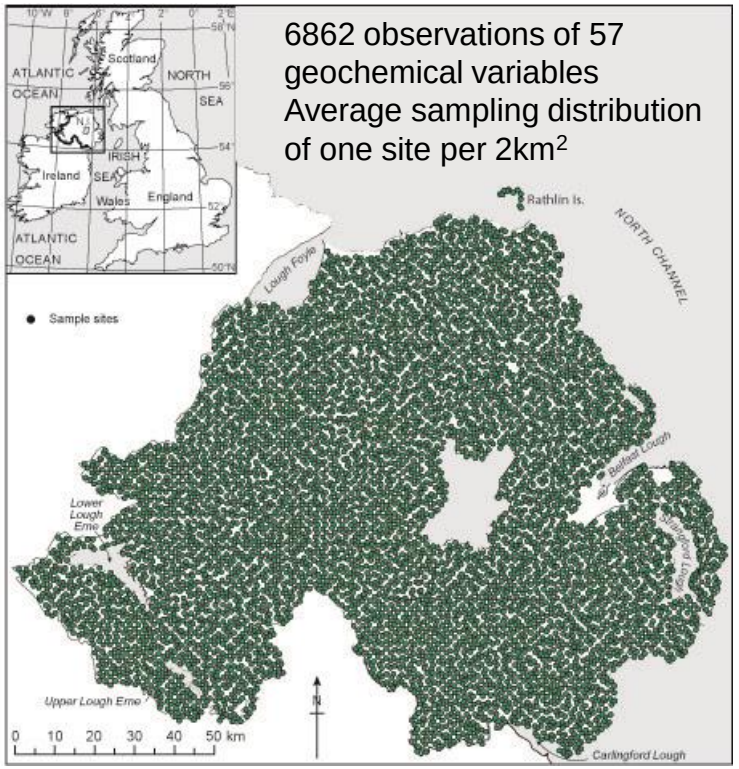

The Tellus geochemical soil survey, Northern Ireland, UK

A guide to the Tellus data. 2013.Young, M. E. and Donald, A. W. (eds). Geological Survey of Northern Ireland (GSNI), Belfast.

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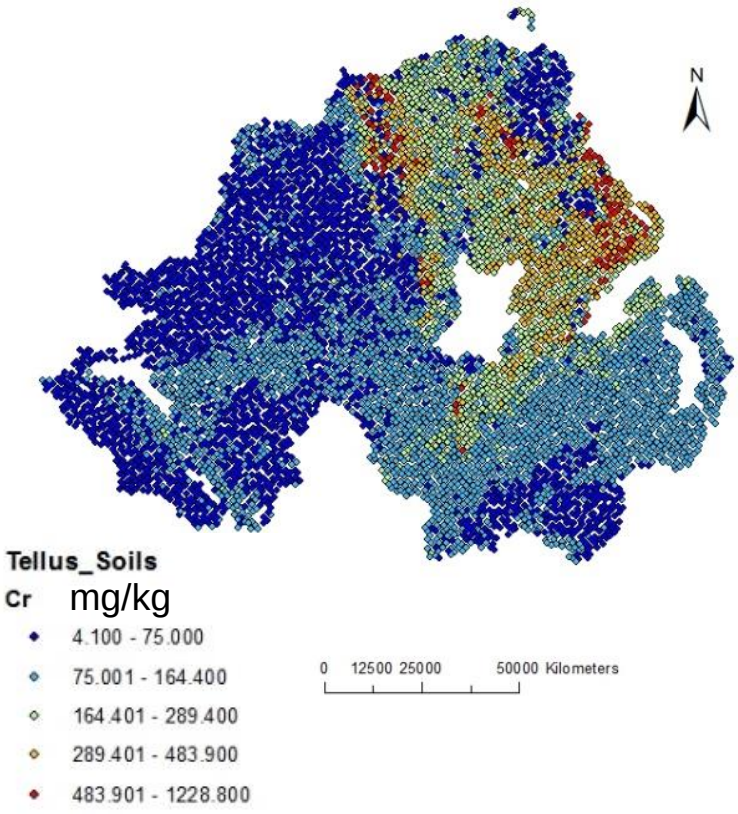
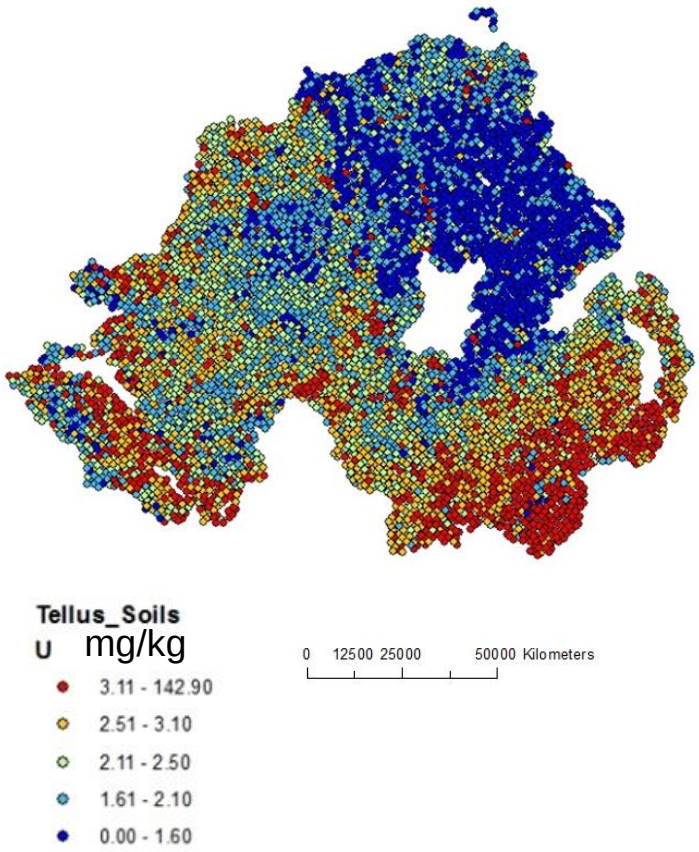
Point maps – the objective ground truth?

It is often thought that raw one-component maps report “what is there”, that they report a sort of “objective ground truth”.





The application of log-ratio techniques

- Ratios between components are unaffected by constant sum closure effects caused by the relative nature of geochemical data (Pawlowsky-Glahn & Buccianti 2011; Egozcue & Pawlowsky-Glahn 2011).
- Several families of log-ratio transformations exist.
- Aitchison (1986) introduced the pairwise log-ratio transformation (pwlr), the additive log-ratio transformation (alr) and the centred log-ratio transformation (clr).
- Egozcue et al. (2003) proposed the isometric log-ratio (ilr) transformation.
- None is inherently better than the other, each has advantages and disadvantages.

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What does the compositional nature of geochemical data mean for using geochemical elements for geogenic radon mapping?

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Need for an analysis approach that honours the compositional nature of the geochemical data and offers an interpretable mapped output

Two approaches are suggested by McKinley et al. (in review):

- Knowledge-driven log-ratios, chosen to highlight certain geochemical relations or to filter known artefacts.
- Data driven approach: supervised and unsupervised methods.
  - Log-contrasts, that employ suitable statistical methods (regression analysis, PCA, clustering of variables, etc.) to extract potentially interesting geochemical summaries.

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A compositional data analysis example

- Balances are simply (normalized) log-ratios of the geometric means of two groups of elements.
- Obtained by an ilr (isometric log ratio) based on balances by choosing a binary hierarchy of association of elements (or a binary partition).

- R package: ‘compositions’ Compositional Data Analysis
- K. Gerald van den Boogaart ; Raimon Tolosana-Delgado (2008).

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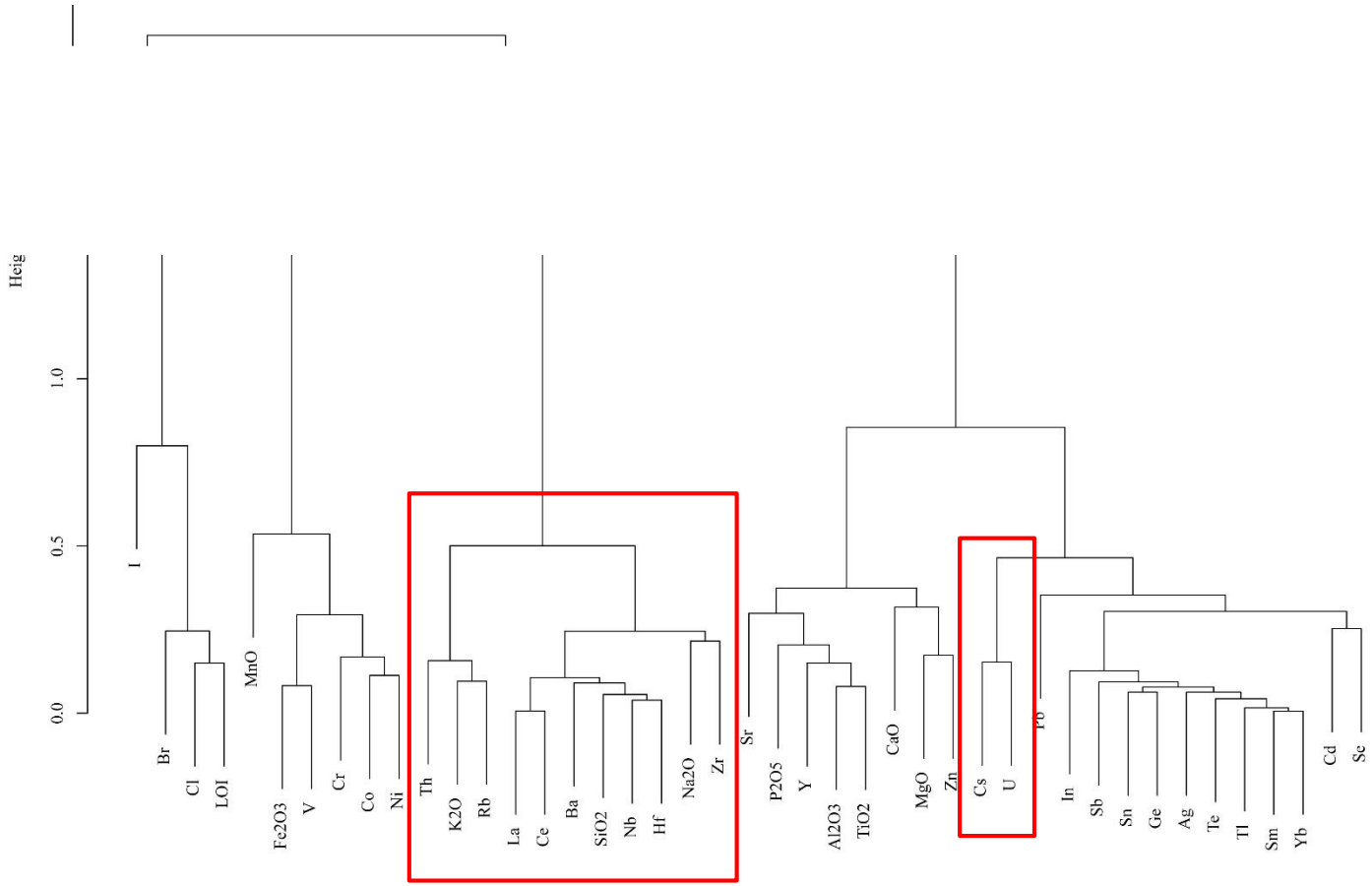
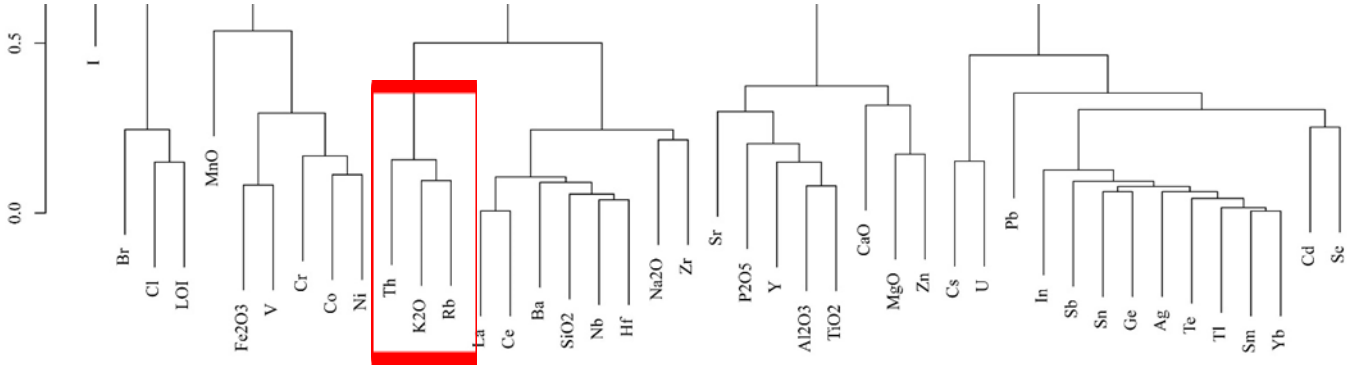
The Cluster Dendrogram



Subcompositions

- For instance the two log-ratios necessary to describe the behaviour of the subcomposition (Th, K_2O, Rb):
- $\xi_1 \propto \ln \frac{K_2O}{Rb}, \qquad \xi_2 \propto \ln \frac{Th}{\sqrt[2]{K_2O \cdot Rb}},$



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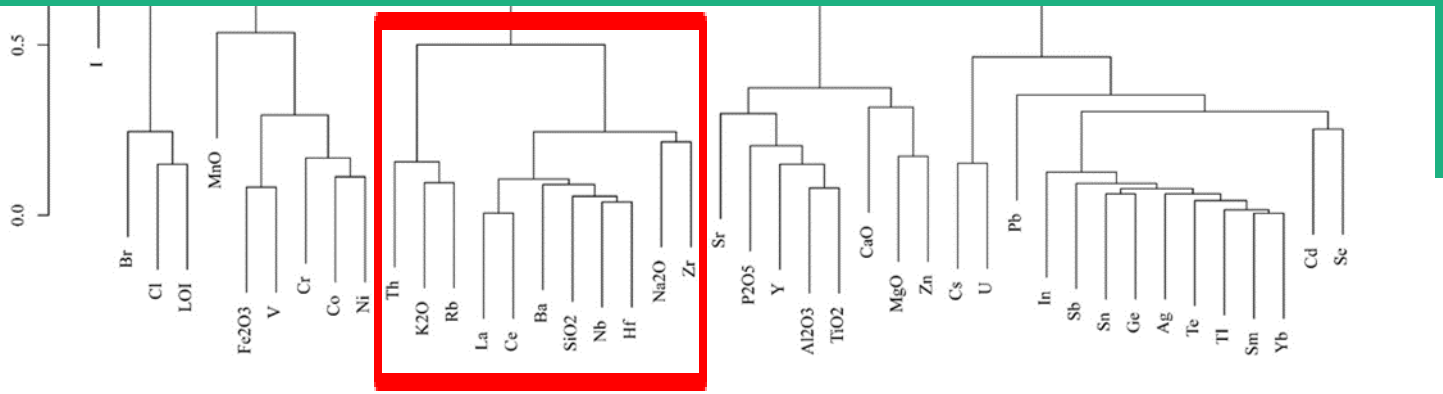

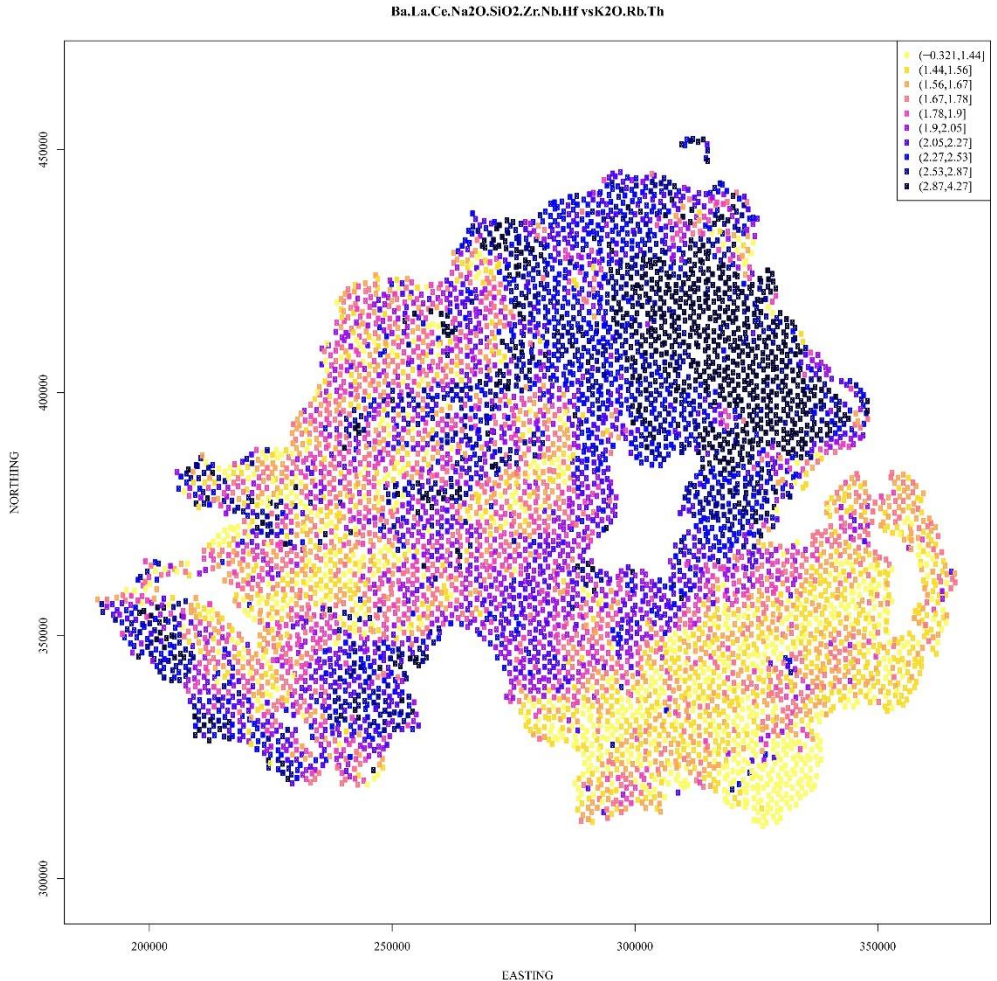

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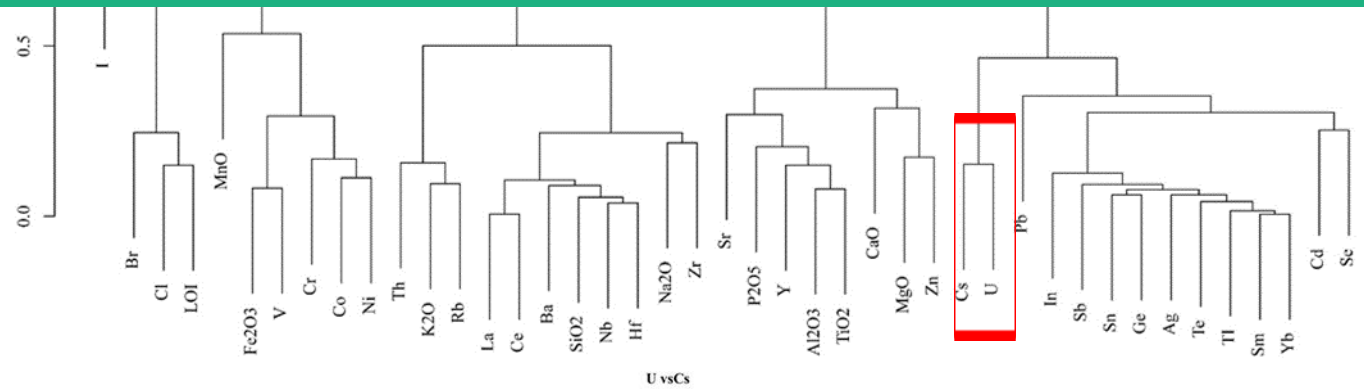

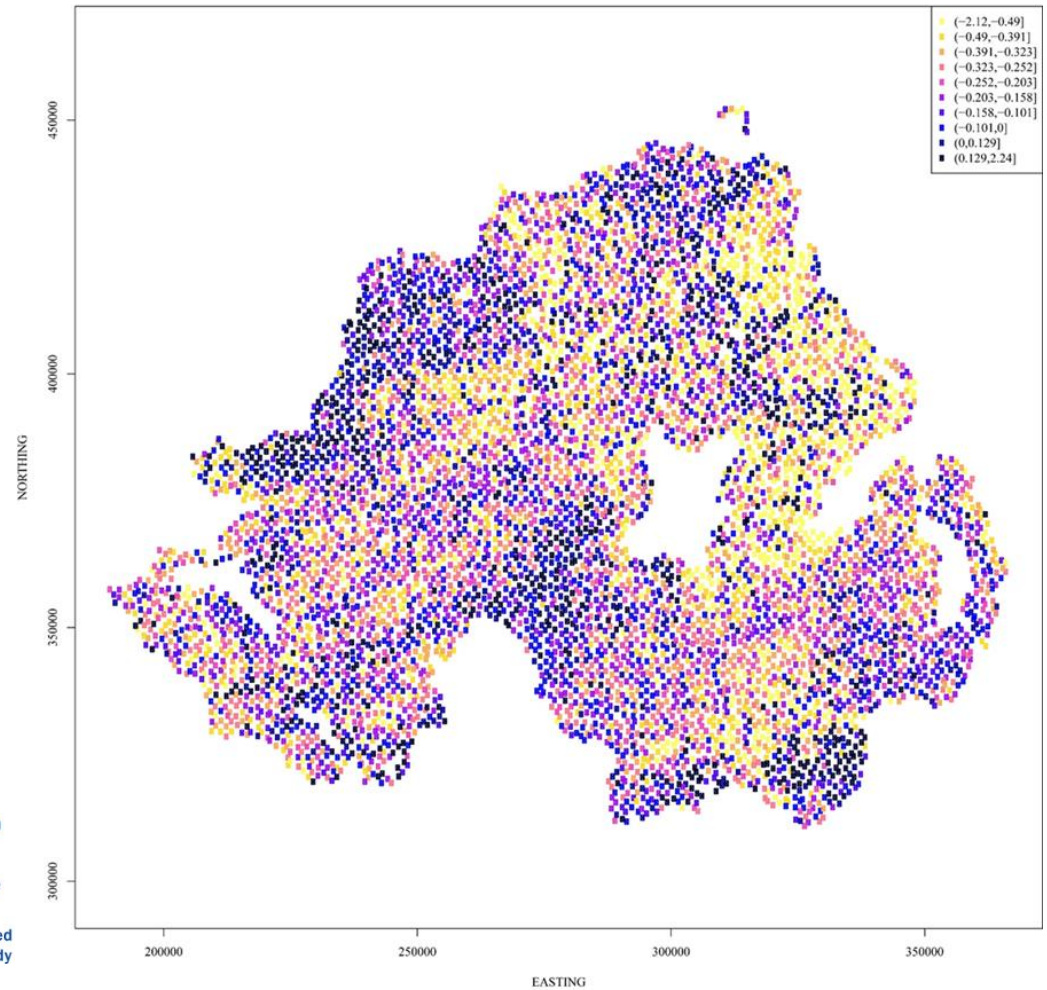

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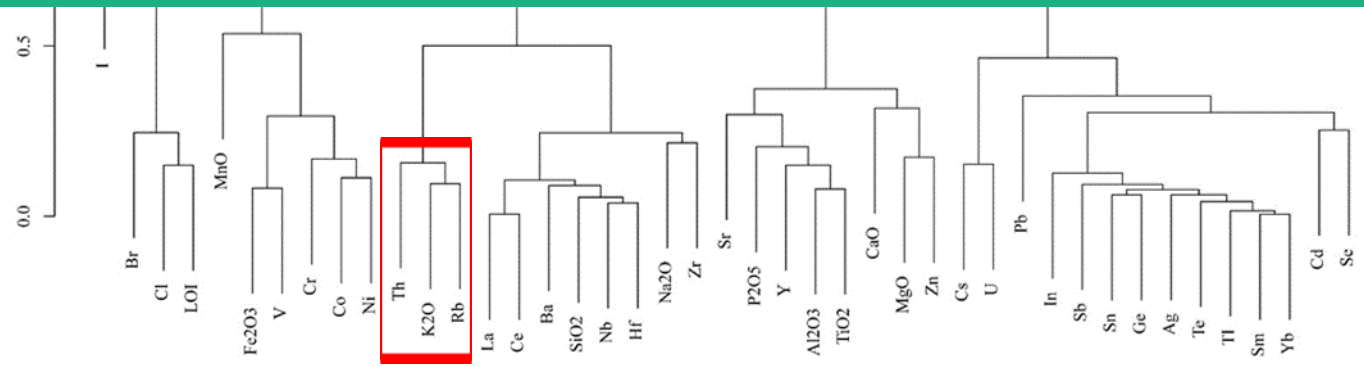
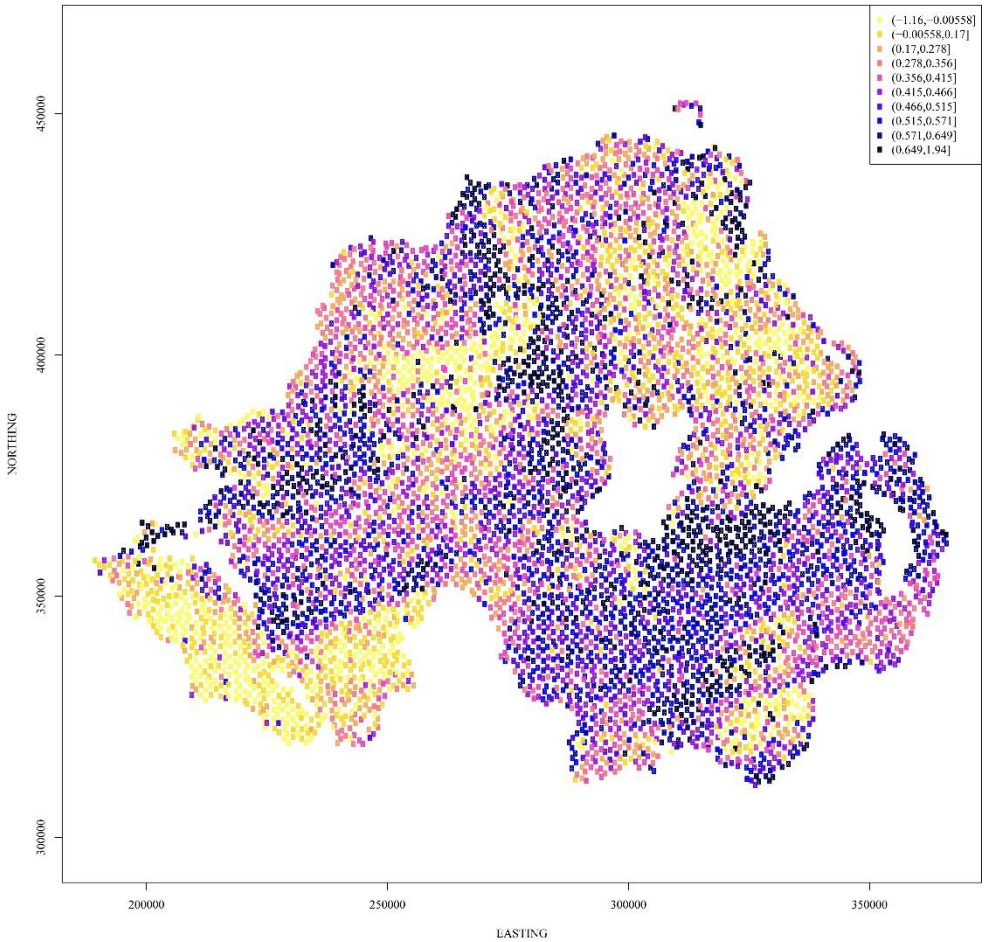


K2O.Rb vsTh



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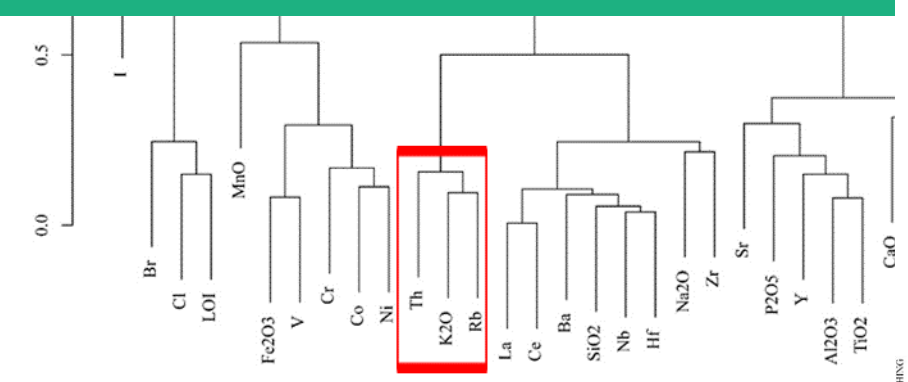
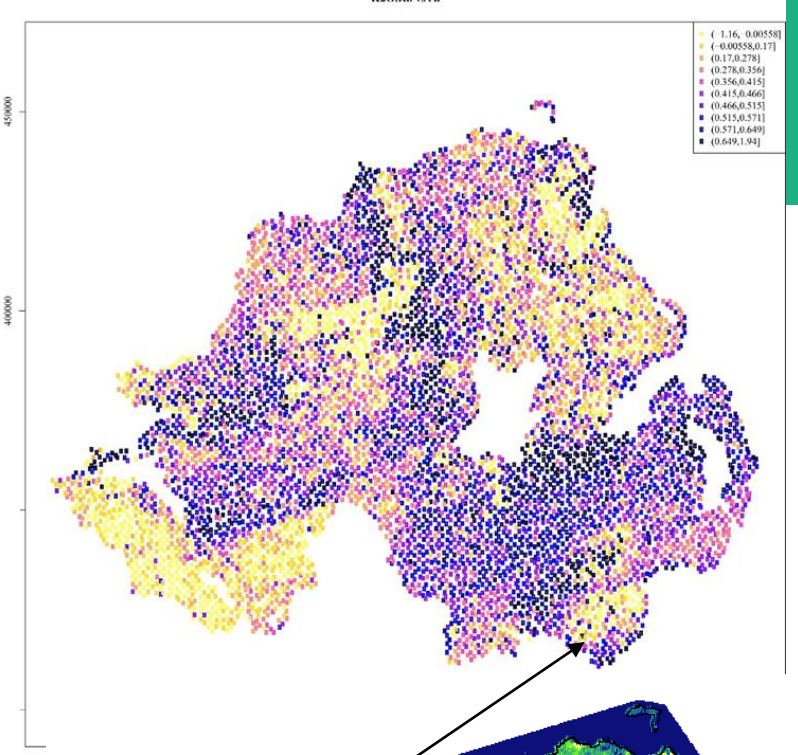
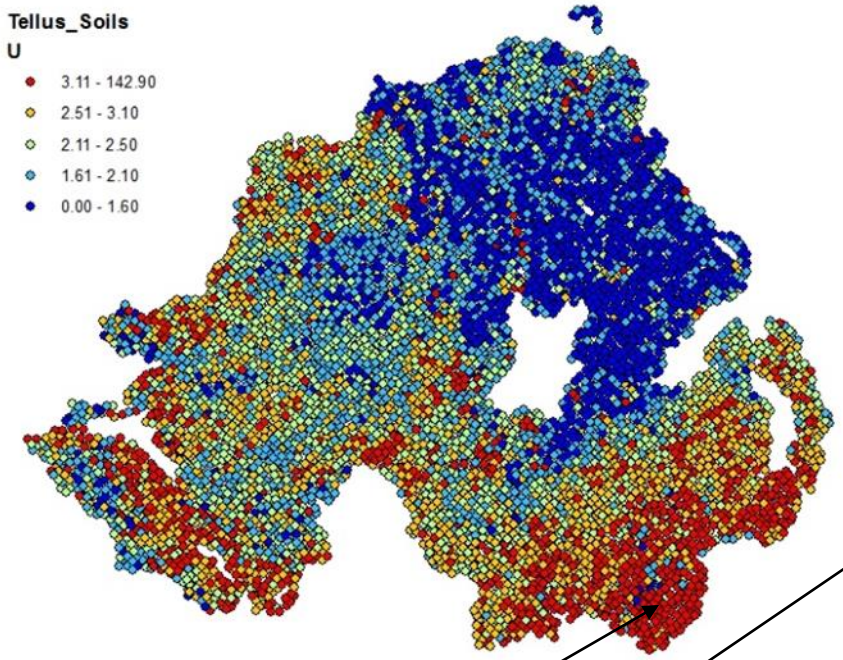
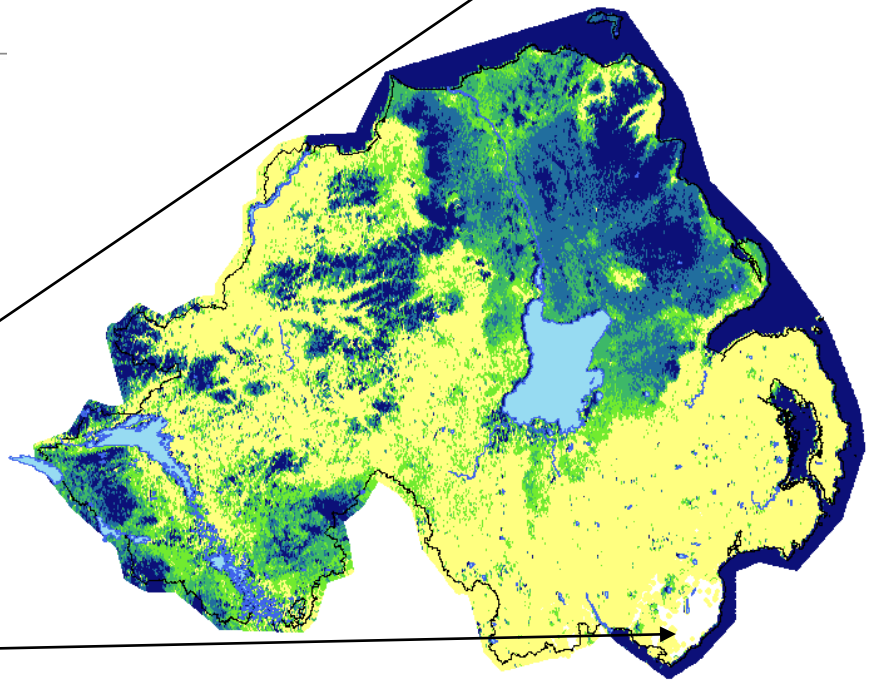




Uranium in soils



Elevated areas – Mourne Mountains



Gamma Radiation Dose rate

Recommendations for using geochemistry data for geogenic radon potential (summarised from McKinley et al in review)

It is suggested to use a chain of enquiry that involves:

- Searching for the appropriate statistical method that can answer the required geological or geochemical question
- whilst maintaining the integrity of the compositional nature of the data;
- applying the required log-ratio transformation and the chosen statistical method;
- and learning to interpret the results.

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Funding and Data providers

EU INTERREG IVA programme Special EU Programmes Body

which is managed by the Special EU Programmes Body in Northern Ireland, the border Region of Ireland and western Scotland

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